

Discrete eigenproblems

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Schrödinger eigenproblems on a discrete interval are further investigated with special attention given to test cases such as the linear and Rosen–Morse potentials. In the former case it is shown that the characteristic function determining the eigenvalues is a Lommel polynomial and considerable space is devoted to these objects. For example it is shown that the continuum limit of the determinant is obtained by a transitional limit of the Lommel polynomials for large order and argument.

Numerical comparisons between discrete approximations and (known) continuum values for the ratio of functional determinants with and without the potential are made and show good agreement, even for small numbers of vertices.

The zero mode problem is also briefly dealt with.

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1. Introduction

In the course of a previous work, [1], investigating the, rather basic, problem of the analogue of the Schrödinger equation on a discretised interval (or ‘path’), Chebyshev polynomials appeared as unperturbed propagators. The use of these polynomials in the context of the free equation occurs in earlier works, [2–4]. In this communication, I wish to enlarge on the technique employed in [1] of replacing the three-term recurrence by a two by two matrix, two-term one, as outlined in the classic Atkinson, [5]. There is nothing new in content, but it has a manipulative advantage, allowing basic properties and computations to be expressed compactly.

In addition to developing this formalism (in sections 2 and 5) I present some numerical studies of particular potentials comparing the ‘exact’ continuum results with the discrete ‘approximations’. I treat the discrete, confined, linear potential in some analytical detail and show that the characteristic polynomial is a Lommel polynomial. These quantities have not had many physical applications and so I present some basic, and not so basic, facts.

2. The recurrences

The basic eigenvalue three-term recurrence, (*e.g.* [6]),

$$y(j+1) + (\lambda - V(j) - 2)y(j) + y(j-1) = 0, \quad (1)$$

subject to two-point boundary conditions, say Dirichlet, Neumann or Robin,

$$\begin{aligned} y(0) &= y(p+1) = 0, & D \\ y(0) &= y(1), \quad y(p) = y(p+1), & N \\ \Delta y(0) &= \alpha y(0), \quad \Delta y(p) = -\beta y(p+1), & R. \end{aligned} \quad (2)$$

at the boundary, $\partial\mathcal{I}$, of the discrete interval, \mathcal{I} , which is comprised of the $(p+2)$ points $j = 0, 1, \dots, p, p+1$. $\partial\mathcal{I} = 0 \cup p+1$.

This is a discrete Sturm–Liouville problem.

$V(j)$ is the potential because (1) can be rewritten as the more familiar looking Laplacian eigenvalue equation,²

$$[-\nabla\Delta + V(j)]y(j) = \lambda y(j). \quad (3)$$

² ∇ is the backwards difference operator. There are many discrete approximations to the continuum $-y''(x) + \bar{V}(x)y(x) = \lambda y(x)$.

As well as the homogeneous equation (3), the inhomogeneous one

$$[-\nabla\Delta + V(j) - \lambda]y(j) = \rho(j). \quad (4)$$

is of interest where $\rho(j)$ is a source density and λ a spectral parameter.

As intimated in the Introduction, it is helpful to recast these three-term relations by two-term matrix ones and I have to use a little space to set this up.

For example (1) (*i.e.* (3)), and (4) can be replaced by the matrix recurrences,

$$\Upsilon(j) = C(x_j)\Upsilon(j-1) \equiv C(j)\Upsilon(j-1) \quad (5)$$

and

$$\Upsilon(j) = C(j)\Upsilon(j-1) + D R(j-1) \quad (6)$$

respectively, with the definitions

$$\Upsilon(j) = \begin{pmatrix} y(j) \\ y(j+1) \end{pmatrix}, \quad R(j) = \begin{pmatrix} \rho(j) \\ \rho(j+1) \end{pmatrix} \quad (7)$$

and

$$C(j) = \begin{pmatrix} 0 & 1 \\ -1 & V(j) + 2 - \lambda \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & \phi(j) \end{pmatrix}. \quad (8)$$

The driving matrix, C , can be split as $C(j) = B(j) - \lambda D(j)$ where,

$$B(j) = \begin{pmatrix} 0 & 1 \\ -1 & V(j) + 2 \end{pmatrix}, \quad D(j) = D = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (9)$$

If Υ_1 and Υ_2 are two general solutions of the difference equation, (5), the constancy of their Casoratian,

$$\tilde{\Upsilon}_1(j) J \Upsilon_2(j) = \det(\Upsilon_1 \otimes \Upsilon_2) \quad (10)$$

follows immediately, where J is the symplectic metric,

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The replacement of a second order difference equation by two, first order ones, organised into matrix form, is the simplest example of the more general case where an n th order equation is replaced by an $n \times n$ matrix equation of the first order. Birkhoff, [7], for example, makes extensive use of this formulation. Milne-Thomson,

[8], §5.3, §12.8, also employs the same technique in the language of continued fractions. See also [9] and the compact discussion in [10] extended in Agarwal, [11].

Taking the discrete interval \mathcal{I} as the archetypal domain, the propagation (5) can be ‘solved’ as,

$$\Upsilon(j) = K(j, j') \Upsilon(j') = K(j, 0) \Upsilon(0),$$

where $\Upsilon(0)$ is the given initial vector and $K(j, j')$ is the forwards propagator,

$$K(j, j') = \theta(j, j') C(j) C(j-1) \dots C(j'+1), \quad (11)$$

which I concentrate on.

Equivalent to (5) is

$$K(j, j') = \delta_{jj'} \mathbf{1} + C(j) K(j-1, j'), \quad (12)$$

incorporating the initial condition $K(j, j) = \mathbf{1}$. In particular, for $K(j) \equiv K(j, 0)$ one has

$$K(j) = \delta_{j0} \mathbf{1} + C(j) K(j-1). \quad (13)$$

In my previous work, I treated the potential, $V(j)$, as a perturbation. This amounts to extracting the factor of $2 - \lambda$ in $C(j)$ which produces a rearrangement of (12) with Chebyshev polynomials as unperturbed propagators. This is formally attractive, but, if all one is interested in is a numerical answer, then a direct iteration of (13) is adequate. Even though it is absolutely equivalent to (1), it is computationally advantageous. Furthermore, in order to implement Dirichlet boundary conditions, say, it is sufficient to find the bottom right-hand component of $K(p+1)$, *i.e.* $\text{Tr}(K(p+1) D)$, and the relevant recurrence is

$$K_D(j) = D \delta_{j0} \mathbf{1} + C(j) K_D(j-1), \quad (14)$$

where $K_D(j) \equiv K(j) D$. This is easily programmed.

3. An explicit example. The linear potential.

In the continuum, Kirsten and McKane, [12], as a simple illustration of the Gel'fand–Yaglom procedure, compute the ratio of Laplacian functional determinants with and without a linear potential, specifically for the operator,

$$L(x) \equiv -\frac{d^2}{dx^2} + \overline{V}(x), \quad (15)$$

with $\overline{V}(x) = b^3 x$. They chose $b = 1$, but I use a general strength.

As is well known, Airy functions arise for such a potential and Kirsten and McKane give, on this basis, 1.085(339648) for the determinant ratio.

I outline some details later in this section but first I give the discrete version of this computation. I proceed to write down the relevant recurrence in scalar form, *i.e.* equation (1) with the potential linear in j , $V(j) = Bj$,

$$y(j+1) + (\lambda - Bj - 2)y(j) + y(j-1) = 0, \quad (16)$$

with, for simplicity, Dirichlet boundary conditions at $j = 0$ and $j = p+1$ according to (2).

One might consider this system as describing the motion of a charged particle in a uniform electric field, confined to a box, *i.e.* interval.

This recurrence is an example of a more general type analysed by Boole, [13], using operator methods and, more analytically, by Barnes, [14], but, again I will not use their results. Rather, in the particular case of (16), I refer, at the moment, to Bleich and Melan, [15], who give a rather detailed treatment of recursions of the form,

$$y(j+1) - \phi(j)y(j) + y(j-1) = 0, \quad (17)$$

i.e. (5) with (8).

Starting from a solution Ansatz suggested by the iteration of (17), or (5), they show that, for a necessarily restricted set of functions, $\phi(j)$, explicit solutions are possible.

In particular a Dirichlet solution for $\phi(j) = A + Bj$ is presented in equation (59) on p.149 in [15]. In my notation $A = 2 - \lambda$ and I set their initial point, η to 0. For the moment, I just quote their forwards solution which transcribes (with some inessential notational adjustments) to ³,

$$y(j, \lambda) = \sum_{k=0}^{j-1} \cos \frac{k\pi}{2} \binom{j - k/2 - 1}{k/2} \prod_{l=1}^{j-k-1} [A + B(k/2 + l)]. \quad (18)$$

I make further comments on this expression in sections 6 and 7 where I relate it to Lommel polynomials.

To give a flavour of the structure of this solution, I compute $y(4, \lambda)$, which corresponds to the terminal value if I choose p to equal 3.

³ I draw attention to the definition of the product symbol in [15] on p.141 and footnote on p.151, which differs from the usual one used here.

Because of the cosine, k can only be even and therefore only 2 or 0 so that,

$$\begin{aligned} y(4, \lambda) &= (2 - \lambda + 2B)((2 - \lambda + B)(2 - \lambda + 3B) - 2) \\ &= -\lambda^3 + \lambda^2(6 + S_1) - \lambda(10 + S_2 + 4S_1) + 4 + 4S_1 + 2S_2 + S_3 - 4B, \end{aligned} \quad (19)$$

where, for comparison purposes, I have defined $v_1 = 1B$, $v_2 = 2B$ and $v_3 = 3B$ as the values of the linear potential Bj at $j = 1, 2, 3$ and also where

$$S_1 = v_1 + v_2 + v_3, \quad S_2 = v_1v_2 + v_1v_3 + v_2v_3, \quad S_3 = v_1v_2v_3. \quad (20)$$

I have done this in order to compare with the expression derived in [1] for a general potential. The comparison is exact if one takes into account the special relation here that $\nabla\Delta v_2 = v_1 - 2v_2 + v_3 = 0$ for a linear potential.

The eigenfunction, for a given eigenvalue, say λ_n , is given by $y(j, \lambda_n)$, (18), where n ranges over p values, say $1 \leq n \leq p$, (setting the terminal point to $j = p+1$).

It is interesting to note that if p is odd, there is always an eigenvalue, halfway along, $\lambda_{(p+1)/2} = 2 + B(p+1)/2$ for which, as is obvious and can be checked, first order perturbation theory is exact.

Finally, from general theory, the ratio of determinants is given by,

$$\overline{\det}(B) \equiv \frac{\det(B)}{\det(0)} = \frac{y(p+1, 0)}{y(p+1, 0)|_{B=0}}, \quad (21)$$

which can be evaluated from (18).

In order to compare with the *continuum* linear potential, $\overline{V} = b^3x$, the strength, B of the discrete potential has to be rescaled. Over the unit interval, one has $B = (b/(p+1))^3$ by dimensions.

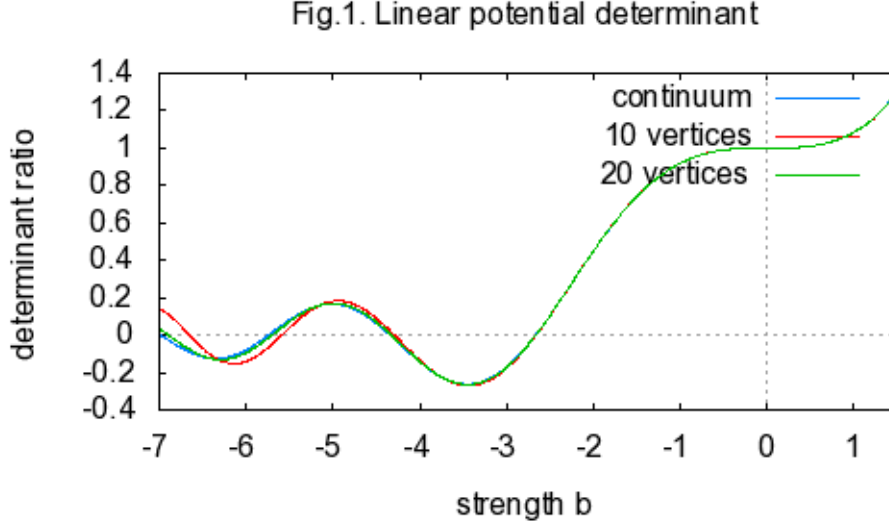
For $b = 1$, I get a determinant ratio value of 1.08533860, choosing $p = 300$.⁴ This is not particularly efficient, but comparison with the continuum value, 1.085339648, demonstrates the validity of the methods. More interesting, perhaps, is that for just one interpolating step, *i.e.* $p = 1$, the value is 1.0625, for $p = 3$ it is 1.07947 while for ten, I find 1.08456, a reasonable approximation.

These results suggests that, if one is prepared to sacrifice a little accuracy, the determinant ratio for any potential can be calculated almost by hand.

Incidentally, for an *attractive* potential ($b < 0$), bound states arise and in Fig.1 I plot the determinant ratio that demonstrates this fact by the zeros. Not so

⁴ In 1.4 secs using the wxMaxima CAS on an Athlon ii x 4 machine.

interestingly, for a repulsive potential, the ratio shows a rapid, monotonic increase. The continuum curve is also shown in the figure.



For the continuum situation, the Gel'fand–Yaglom function for the potential $b^3 x$ is, *cf* [12],

$$y_1(x) = \frac{\pi}{b} (\text{Bi}(0) \text{Ai}(bx) - \text{Ai}(0) \text{Bi}(bx)) , \quad (22)$$

and yields the ratio of determinants,

$$\frac{\pi}{b} (\text{Bi}(0) \text{Ai}(b) - \text{Ai}(0) \text{Bi}(b)) , \quad (23)$$

which is also plotted in Fig.1. The figure also shows that the discrete approach is good for smallish strengths, b , as expected since it is a perturbation-like method yielding a finite polynomial (in b) approximation for the Airy expression, (22). This is discussed further in sections 6 and 7.

4. The Rosen–Morse potential

Bound states also arise for the Pöschl–Teller, hyperbolic potential,

$$\overline{V}(x) = -\frac{l(l+1)}{\cosh^2(x)} , \quad (24)$$

confined to a box, as considered by Dunne, [16].

From its quantum mechanical origins in molecular physics, the strength, l , is usually taken to be integral, but can, in fact, be any real number, in which case it

might be preferable to use the variable $\bar{l} = l + 1/2$. I will still employ l but refer to (24) as the Rosen–Morse potential (*e.g.* Kleinert, [17], Flügge, [18]).

Two particular solutions of the equation, $L(x) \psi(x) = 0$,⁵ are the Legendre functions, $P_l(\tanh x)$ and $Q_l(\tanh x)$, constituting a fundamental set. I choose the interval $-1/2 \leq x \leq 1/2$ as domain so that I can give the Gel’fand–Yaglom function as written down by Dunne,

$$\psi_{GY}(x) = P_l(-\tanh 1/2) Q_l(\tanh x) - P_l(\tanh 1/2) Q_l(-\tanh x)$$

so that the ratio of determinants, with and without \bar{V} , is

$$\overline{\det}_C(l) = P_l(-t) Q_l(t) - P_l(t) Q_l(-t) \quad (25)$$

where $t = \tanh 1/2 \approx 0.46211715726$. Properties of the Legendre functions check that $\overline{\det}_C(l)$ is symmetrical in \bar{l} , as must be, and one need compute it only for positive \bar{l} , *i.e.* $l \geq -1/2$.

In terms of functions of the first kind, I find,

$$\overline{\det}_C(l) = \frac{\pi}{\sin \pi l} (P_l(-t)^2 - P_l(t)^2) \quad (26)$$

which is easily calculated using Gauss’ hypergeometric form, say,

$$P_l(t) = {}_2F_1(-l, 1+l; 1; (1-t)/2).$$

Near integral l , the numerics become uncertain. But for l actually integral, the ratio of determinants, (25), can be expressed purely in terms of the polynomials, P_l ,

$$\overline{\det}_C(l) = (-1)^l P_l \left(P_l - 2 \sum_{m=1}^l \frac{1}{m} P_{m-1} P_{n-m} \right), \quad l \in \mathbb{Z}, \quad (27)$$

which is a polynomial in $\tanh 1/2$ and provides a check of the numbers. As an exercise, one could use these values as the basis of an interpolation.

Turning now to the discrete calculation, the formula I use is that developed in [1]. For $p = 3$, an interval with three interior vertices and step size $h = 1/4$, the determinant ratio is,

$$\overline{\det}_D(l) = 1 + \frac{1}{4}(3S_1 + 2S_2 + S_3 + v_2), \quad (28)$$

⁵For simplicity, I set the mass equal to zero.

where the S_i are given by (20) with $v_j \equiv V(j)$. (Refer to (3)). This is to be compared, numerically, with (26).

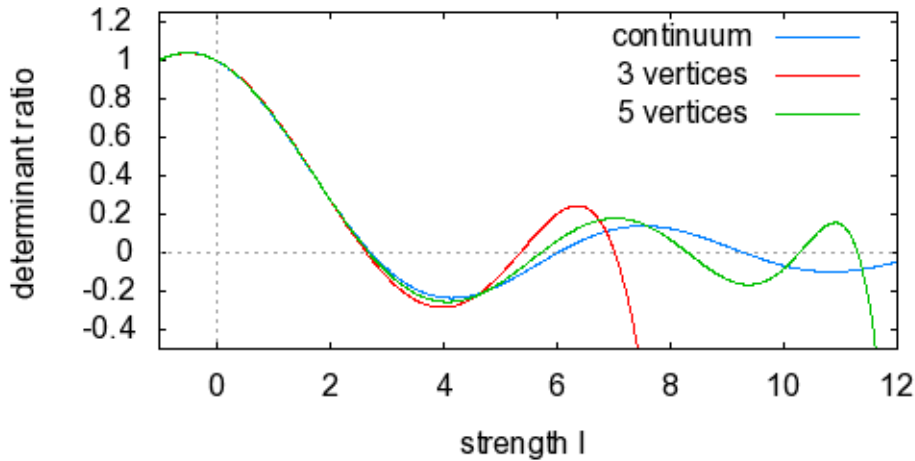
On this side of the calculation, I use the interval 0 to 1 so that the discrete potential corresponding to (24) is given by

$$V(j) = -\frac{h^2 l(l+1)}{\cosh^2(hj - 1/2)}$$

and the evaluation of (28) is relatively elementary. The results are presented graphically in fig.2, where I have also displayed the 5 vertex values and the continuum, ‘exact’ curve, based on (26).

The figure shows again that the discrete approach is good for smallish strengths, l . It yields a finite polynomial (in l , even in \bar{l}) approximation for the Legendre expression, (25). The exact curve oscillates for ever and, while a finite polynomial cannot do so, it follows fairly well, for a decent range of l . Note also that, for a repulsive potential, the ratio is bigger than one.

Fig.2. Rosen-Morse determinant



The zeros of the curves occur when bound states appear as the well deepens.

5. Analytical extensions

So far it has been assumed that label j takes just integral values. However in classical finite difference theory, *e.g.* Boole, [13], this is only a particular case of a more general situation where one deals with functions $y(x)$ of a variable, x (real or complex) satisfying a difference equation, say,

$$y(x+1) - \phi(x)y(x) + y(x-1) = 0, \quad (29)$$

as a relevant, typical example. In accordance with my previous formalism, I write this, with, therefore, some repetition from section 2, as,

$$\Upsilon(x) = C(x)\Upsilon(x-1) \quad (30)$$

with

$$\Upsilon(x) = \begin{pmatrix} y(x) \\ y(x+1) \end{pmatrix}, \quad (31)$$

and

$$C(x) \equiv \begin{pmatrix} 0 & 1 \\ -1 & \phi(x) \end{pmatrix}. \quad (32)$$

Assuming some starting point, $x = x_0$, the general solution of (30) is

$$\begin{aligned} \Upsilon(x) &= C(x)C(x-1) \dots C(x_0+1)\Upsilon(x_0) \\ &= K(x, x_0)\Upsilon(x_0) \end{aligned} \quad (33)$$

where $\Upsilon(x_0)$ can be considered as an arbitrary constant vector, say Ω .

For a particular x_0 , the domain of x is determined, but one can consider x_0 to change, and with it, the domain of x , (see *e.g.* Boole, [13], p.102, Levy and Lessman, [19], pp.89+) (always, however, with $x - x_0$ integral). This can be accommodated by making the constant, Ω , a function,

$$\Omega(x) = \begin{pmatrix} \varpi_\alpha(x) \\ \varpi_\beta(x) \end{pmatrix},$$

where the ϖ_i are arbitrary unit periodics, Böhmer, [20], [15], §26, [19], [8], §11.1, (*e.g.* $\varpi_i(x_0) = \varpi_i(x)$) so that the general solution, (33), is,

$$\begin{aligned} \Upsilon(x) &= C(x)C(x-1) \dots C(x_0+1)\Omega(x_0) \\ &= K(x, x_0)\Omega(x_0) \\ &= \varpi_\alpha(x)\Upsilon_\alpha(x) + \varpi_\beta(x)\Upsilon_\beta(x), \end{aligned} \quad (34)$$

where,

$$\Upsilon_\alpha(x) = K(x, x_0)\boldsymbol{\alpha}, \quad \Upsilon_\beta(x) = K(x, x_0)\boldsymbol{\beta}, \quad (35)$$

with the standard basic vectors,

$$\boldsymbol{\alpha} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (36)$$

For example, Dirichlet initial conditions require $\varpi_\alpha(x_0) = 0$.

The solution (34) is just the general solution to the second order difference equation (29), a standard construct, *e.g.* Levy and Baggott, [21], Birkhoff, [7].

The basis, Υ_α and Υ_β is a *canonical* one (*e.g.* Lakshmikantham and Trigiante, [10], Lemma 2.1.1).

Υ_β coincides with Atkinson's *standard solution*, $y_n(\lambda)$, [5], equns. (4.1.4), (4.1.5) and Υ_α with the standard solution, $z_n(\lambda)$, equns. (4.2.6), (4.2.8).

As a non-trivial example, the solution (18) to (17), corresponds to the Dirichlet solution $\Upsilon_\beta(j)$ because $y(0, \lambda) = 0$ and $y(1, \lambda) = 1$. In the following section, I enlarge on this solution.

The constancy of the Casoratian, (10), now becomes the statement that it is a unit periodic,

$$\tilde{\Upsilon}_1(x) J \Upsilon_2(x) = \varpi(x),$$

where Υ_1 and Υ_2 are two *general* solutions of the difference equation, (30) each of the form (34), say.

6. Bessel functions

I return to a consideration of the confined linear potential of section 3, which forms an interesting, if somewhat specific, case but with connections to some special functions.

The analysis of the second order equation by Barnes and by Bleich and Melan, proceeds from the classic form of the recurrence, (29), so I present their results accordingly, despite my preference for the matrix form.

The equation in question is (*cf* (16)), ⁶

$$y(x+1) - (Bx+A)y(x) + y(x-1) = 0, \quad (37)$$

which, treated using the textbook Laplace method, ⁷ yields two independent solutions as contour integrals coinciding, to a simple factor, with Bessel functions,

$$\begin{aligned} y^{(1)}(x) &= (-1)^{x+A/B} J_{-(x+A/B)}(2/B) = J_{-(x+A/B)}(-2/B) \\ y^{(2)}(x) &= J_{(x+A/B)}(2/B), \end{aligned} \quad (38)$$

⁶ This is recognised as a recurrence relation for Bessel functions but it is not necessary to do so at this time.

⁷ A simple discussion is given in the elegant little book by Miller, [9].

and the general solution is

$$y(x) = \varpi_1(x) y^{(1)}(x) + \varpi_2(x) y^{(2)}(x). \quad (39)$$

If $\xi = x + A/B$ is an integer then these two solutions are equivalent and, in the usual fashion, a second solution is obtained by a limiting process, $\xi \rightarrow n$, on a Bessel function of the second kind, due to Weber and Schläfli,

$$Y_\xi(z) = \cot \xi \pi J_\xi(z) - \frac{1}{\sin \xi \pi} J_{-\xi}(z), \quad (40)$$

which satisfies the difference equation (29) as it is of the form (39).

As an application, return to the conventional case when $x = j \in \mathbb{Z}$ with the previously used discrete interval, \mathcal{I} , as domain and attempt to recover earlier results, such as (18). Thus, apply D conditions at $j = 0$ and $j = p + 1$. This produces the non-local Casorati determinant condition,

$$\begin{vmatrix} y^{(1)}(0) & y^{(2)}(0) \\ y^{(1)}(p+1) & y^{(2)}(p+1) \end{vmatrix} = 0, \quad (41)$$

which is just the vanishing of the Dirichlet solution,

$$y(x, \lambda) = y^{(2)}(0) y^{(1)}(x) - y^{(1)}(0) y^{(2)}(x)$$

at the terminal point, $x = j = p + 1$.

Inserting the explicit functions, (38) gives the quantity,⁸

$$W(\nu, p) \equiv J_{-\nu} J_{p+1+\nu} - (-1)^{p+1} J_{-(p+1+\nu)} J_\nu = 0, \quad p \in \mathbb{Z}, \quad (42)$$

where $\nu \equiv A/B$ and the arguments of the Bessel functions are all $2/B \equiv z$. I have dropped inessential, common overall constants and leave the dependence of W , which is hereby defined, on z implied, until later.

The characteristic equation, (41), in λ (remember, $A = 2 - \lambda$) provides the eigenvalues through its roots, and is easily computable since, in this case, two independent solutions are known.

The aim, then, is to show that the Casoratian, (41), is proportional to a finite polynomial in ν of order p , *cf* (18). This can be done via the series form of the Bessel functions in (42). Of course, it is to be anticipated that the Casoratian

⁸ The relation is $y(p+1, \lambda) \propto (-1)^\nu W(\nu, p)$.

vanishes when ν is an integer for then the two Bessel functions are proportional. To allow for this, it is convenient to consider the normalised Casoratian,⁹

$$\overline{W}(\nu, p) \equiv \frac{W(\nu, p)}{W(\nu, 0)},$$

which removes the relevant factor.

A standard formula is,¹⁰

$$W(\nu, 0) = J_{-\nu} J_{1+\nu} + J_{-1-\nu} J_{\nu} = -\frac{B}{\pi} \sin \nu \pi. \quad (43)$$

I give the calculation and refer to comments in sections 7 and 8. The composition relation is used to give the series,

$$J_{-\nu} J_{p+1+\nu} = \sum_{n=0}^{\infty} \frac{(-1)^n B^{-(2n+p+1)} (p+n+2)_n}{n! \Gamma(n+1-\nu) \Gamma(p+\nu+n+2)}$$

$$J_{\nu} J_{-p-1-\nu} = \sum_{n=0}^{\infty} \frac{(-1)^n B^{-(2n-p-1)} (n-p)_n}{n! \Gamma(n+1+\nu) \Gamma(n-p-\nu)}.$$

In the combination, (42), most of the terms cancel, leaving the finite sum,

$$W(\nu, p) = \sum_{n=1}^{p+1} \binom{p+1-2n}{-n} \frac{(-1)^n B^{-(p+1-2n)}}{\Gamma(-\nu-n+1) \Gamma(p-n+\nu+2)} \quad (44)$$

Part of the summation range gives zero because $\binom{p+1-2n}{-n} = 0$, if $n \leq (p+1)/2$.

I give the details that turn (44) into (18), up to a factor. The Gamma functions combine as,

$$\begin{aligned} \frac{1}{\Gamma(-\nu-n+1) \Gamma(p-n+\nu+2)} &= \frac{(\nu+p-n+2) \dots (\nu+n-1)}{\pi} \sin \nu \pi \\ &= \frac{(A+B(p-n+2)) \dots (A+B(n-1))}{\pi B^{2n-p-2}} \sin \nu \pi \end{aligned} \quad (45)$$

and the normalised Casoratian is,

$$\overline{W}(A, B, p) = \sum_{n=1}^{p+1} \binom{p+1-2n}{-n} (-1)^{n+1} (A+B(p-n+2)) \dots (A+B(n-1)), \quad (46)$$

⁹ An alternative procedure is given in the next section.

¹⁰ $p=0$ means there are no (internal) vertices.

The number of brackets being $(p - 2s)$.

I have changed arguments to allow for the z dependence. Thus, $\overline{W}(A, B, p) \equiv \overline{W}(\nu, p)(z)$.

The change of summation variable to,

$$k = 2(p + 1 - n),$$

then yields agreement with (18) (if j is chosen to be the end boundary point, $p + 1$) since,

$$\binom{p + 1 - 2n}{-n} = (-1)^{p+1-n} \binom{n-1}{2n-p-2}.$$

Bleich and Melan's solution, (18) has thus been obtained by a more direct and particular route.

Finally the trivial transformation of summation variable $s = p + 1 - n$ converts (46) into, the simpler-looking form,

$$\overline{W}(A, B, p) = (-1)^p \sum_{s=0}^{<(p+1)/2} \binom{p-s}{s} (-1)^s (A + B(p-s)) \dots (A + B(s+1)), \quad (47)$$

where the number of brackets is equal to $(p - 2s)$.

The case $p = 1$,

$$J_{\nu+2}(z) J_{-\nu}(z) - J_{-(\nu+2)}(z) J_{\nu}(z) = -\frac{4(\nu+1) \sin \nu\pi}{\pi z^2},$$

is given in Gray and Matthews, [22], p.241, Ex.1. Other examples are,¹¹

$$\begin{aligned} J_{\nu+3}(z) J_{-\nu}(z) + J_{-(\nu+3)}(z) J_{\nu}(z) &= \frac{2(z^2 - 4(\nu+1)(\nu+2)) \sin \nu\pi}{\pi z^3} \\ J_{\nu+4}(z) J_{-\nu}(z) - J_{-(\nu+4)}(z) J_{\nu}(z) &= -\frac{8(\nu+2)(z^2 - 2(\nu+1)(\nu+3)) \sin \nu\pi}{\pi z^4}. \end{aligned} \quad (48)$$

One could regard the solution (18) as an alternative source of these results which actually are most easily obtained by direct iteration of (37) to give $\Upsilon_2(j)$ of (35) as described in the next section.

I now place these evaluations in a more general and historic setting.

¹¹ For odd p , the vanishing of the overall factor $(\nu + (p + 1)/2)$ corresponds to a cancellation between the two terms on the left-hand side which does not require using $J_n = J_{-n}$.

7. Lommel polynomials

There is no obligation to identify solutions of the recurrence equation, (37), specifically with Bessel functions but making the identification saves a lot of effort due to an extensive literature. For example, the algebra leading to (44), and the further extraction of the factor $\sin \nu \pi$, is well known. What I have termed the normalised Casoratian is a Lommel polynomial (Lommel, [23], Nielsen [24], Graf and Gubler, [25], Watson, [26]) as I now show.

Lommel defined the polynomials, R , from the iteration of the particular Bessel recurrence,

$$F_{\xi+1}(z) = \frac{2\xi}{z} F_{\xi}(z) - F_{\xi-1}(z) \quad (49)$$

specifically for $F_{\xi}(z) = J_{\xi}(z)$ (not the only choice).

Iteration yields the formal solution in terms of two initial values as the reduction formula,¹²

$$F_{\xi+n}(z) = R^{\xi-1,n}(z) F_{\xi}(z) - R^{\xi,n-1}(z) F_{\xi-1}(z),$$

i.e.

$$F_{\xi}(z) = R^{\xi-n-1,n}(z) F_{\xi-n}(z) - R^{\xi-n,n-1}(z) F_{\xi-n-1}(z), \quad (50)$$

where, to confirm the connection with my previous notation in (37), $z = 2/B$, $\xi = x + A/B$ and $y(x, A, B) = F_{x+A/B}(2/B)$. I have included the parameters A and B in the $y(x)$. Either ξ or x can be used as the current, discrete coordinate.

Writing (50) in terms of the initial point ξ_0 , *i.e.* eliminating $n = \xi - \xi_0 - 1$,

$$F_{\xi}(z) = R^{\xi_0, \xi-\xi_0-1}(z) F_{\xi_0+1}(z) - R^{\xi_0+1, \xi-\xi_0-2}(z) F_{\xi_0}(z). \quad (51)$$

Comparison with (35) shows that $R^{\xi_0, \xi-\xi_0-1}(z)$ corresponds to the β , or Dirichlet, solution, and $-R^{\xi_0+1, \xi-\xi_0-2}(z)$ to the α one, as functions of ξ . Checking this requires use of Graf's relation, [25],

$$R^{\nu, -n-1} = -R^{\nu-n, n-1}$$

which implies $R^{\nu, -1} = 0$ and $R^{\nu, -2} = -1$ *e.g.* [25], p.103.

Lommel deduced the actual form of the polynomials, $R^{\xi,n}(z)$, by an inductive procedure repeated by Graf and Gubler, [25] vol.1 chap.1 §2. A simpler method,

¹² I use Nielsen's notation, [24], which is the same as that of Graf and Gubler, [25], who write $\frac{\xi}{P_n}$. It differs from Lommel's and Watson's only in the ordering of the indices and a shift of unity in ξ .

e.g. Nielsen [24], is that give in section 5, since easy algebra leads to Lommel's equation,

$$J_{-\nu}(z) J_{\nu+p+1}(z) + (-1)^p J_{\nu}(z) J_{-\nu-p-1}(z) = -\frac{2 \sin \pi \nu}{\pi z} R^{\nu,p}(z), \quad (52)$$

and the left-hand side can be evaluated from the known series form of $J_{\nu}(z)$. The details in section 5 are, more or less, just a rewriting of Nielsen's algebra and I also give the standard result from this old literature, [23], [24],

$$R^{\nu,p}(z) = \sum_{s=0}^{<(p+1)/2} \frac{(-1)^s (p-s)!}{s!} \binom{\nu+p-s}{p-2s} \left(\frac{2}{z}\right)^{p-2s}, \quad (53)$$

identical to (47).

A comparison of (52) with (42) gives the connection,

$$W(\nu, p) = -\frac{2 \sin \pi \nu}{\pi z} R^{\nu,p}(z), \quad z = 2/B,$$

and the normalised Casoratian is then identical to the Lommel polynomial,

$$\overline{W}(\nu, p) = R^{\nu,p}(z),$$

for non-integral ν . This extends to integral ν by continuity since $R^{n,p}$ is *uniquely* defined (*cf* Watson, [26] §9.61).

The classic result, (43), is a consequence of the general (52) for $p = 0$ together with the explicit form of the $R^{\nu,p}$, although it can be established independently.

In order to regain the notation of (37), ν must be set equal to A/B , and z to $2/B$ and (53) yields the most explicit formula (47), as in section 5. (See below.)

Actually, the passage to integral ν is best approached using the second kind functions, Y_{ν} . Simple algebra using (40) shows that (52) is replaced by the more elegant,

$$\frac{2}{\pi z} R^{\nu,p}(z) = Y_{\nu}(z) J_{\nu+p+1}(z) - J_{\nu}(z) Y_{\nu+p+1}(z) = \begin{vmatrix} Y_{\nu} & Y_{\nu+p+1} \\ J_{\nu} & J_{\nu+p+1} \end{vmatrix}, \quad (54)$$

also due to Lommel, [24]. This will play a role later in the continuum limit.

8. Lommel polynomials as orthogonal polynomials

First a few words regarding variables are relevant here. The variables that provide the standard form of the Lommel polynomials, *i.e.* equation (53), are z and ν related to the ‘physical’ variables $A = 2 - \lambda$ and B where λ is the eigenvalue and B the strength of the (linear) potential, by $\nu = A/B$ and $z = 2/B$, as stated earlier, so that

$$\nu = \frac{2 - \lambda}{B} = \frac{z}{2}(2 - \lambda)$$

In terms of A and B separately, (47) provides the expression for Lommel polynomials. It shows that they are polynomials in both A and B or extracting factors of A or of B , polynomials in B/A or $A/B = \nu$. Here I am interested in polynomials in $A = 2 - \lambda$, or equivalently for fixed B , in ν .

At this point, it is convenient to list a few Lommel polynomials,¹³

$$\begin{aligned} R(\nu, 1) &= (\nu + 1) \left(\frac{2}{z} \right) \\ R(\nu, 2) &= (\nu + 2)(\nu + 1) \left(\frac{2}{z} \right)^2 - 1 \\ R(\nu, 3) &= (\nu + 3)(\nu + 2)(\nu + 1) \left(\frac{2}{z} \right)^3 - 2(\nu + 2) \left(\frac{2}{z} \right) \\ R(\nu, 4) &= (\nu + 4)(\nu + 3)(\nu + 2)(\nu + 1) \left(\frac{2}{z} \right)^4 - 3(\nu + 3)(\nu + 2) \left(\frac{2}{z} \right)^2 + 1 \end{aligned} \tag{55}$$

together with the associated recursion (due to Lommel, [23]) [24], p.54, [25] p.102,

$$R(\nu, p + 2) = \frac{2(p + \nu)}{z} R(\nu, p + 1) - R(\nu, p). \tag{56}$$

By classic, general theory, the $y(j, \lambda)$ of (18), or equivalently the \overline{W} of (46) (with $A = 2 - \lambda$ and $p + 1$ reset to j), *i.e.* the Lommel polynomials, R , form a finite set of explicit orthogonal polynomials (in λ , or ν) concentrated on the eigenvalues, λ_n or ν_n , *e.g.* Atkinson, [5].

For p vertices, orthogonality reads

$$\sum_{j=1}^p R(\nu, j - 1) R(\nu', j - 1) = 1 + \sum_{j=2}^p R(\nu, j - 1) R(\nu', j - 1) = N(\nu) \delta_{\nu\nu'} \tag{57}$$

¹³ There is a misprint on p.102 in [25]. I have temporarily changed notations so that $R(\nu, p) \equiv R^{\nu, p}(z)$.

where ν and ν' are eigenvalues determined by the vanishing of $R(\nu, p)$.

It is interesting to confirm this relation. As a numerical example, take $p = 2$. The eigenvalue equation is then

$$(\nu + 1)(\nu + 2) - \frac{1}{4}z^2 = 0 \quad (58)$$

and (57) reads

$$1 + \frac{4}{z^2}(\nu + 1)(\nu' + 1) = 0, \quad \nu \neq \nu' \quad (59)$$

and

$$1 + \frac{z^2}{4}(\nu + 1)^2 = N(\nu). \quad (60)$$

Using $(\nu + 1)$ as the variable, the product of eigenvalues is, from (58), $-z^2/4$ and (59) is readily verified. (60) fixes the normalisation for orthonormality.

More complicated is the case of $p = 3$. Orthogonality is now

$$1 + \frac{4}{z^2}(\nu + 1)(\nu' + 1) + \left(\frac{4}{z^2}(\nu + 2)(\nu + 1) - 1 \right) \left(\frac{4}{z^2}\nu' + 2)(\nu' + 1) - 1 \right) = 0 \quad (61)$$

From (55) the eigenvalue equation $R(\nu, 3) = 0$ has a solution $\nu = -2$, as mentioned before, and, for simplicity, I set one eigenvalue, $\nu' = -2$ so that (61) reads,

$$1 - \frac{4}{z^2}(\nu + 1) + 1 - \frac{4}{z^2}(\nu + 2)(\nu + 1) = 0$$

which reduces to

$$(\nu + 3)(\nu + 1)\frac{2}{z^2} - 1 = 0, \quad (62)$$

i.e. the equation determining the other two roots of $R(\nu, 3) = 0$ and the confirmation is complete. A similar mechanism works for any odd p .

Showing that (61) holds for solutions of (62) is more complicated.

9. The continuum limit

In this section I show how to derive the continuum determinant ratio, (23), from the above discrete expressions.

I denote by h the path step, $h = 1/(p + 1)$, and seek to let $h \rightarrow 0$, particularly in (54). As noted earlier, the strength, B , of the discrete linear potential is related to b^3 , the strength of the continuum linear potential by $B = (b/(p + 1))^3 = (bh)^3$. Then the argument, $z = 2/(bh)^3 \rightarrow \infty$.

Since I am interested only in the determinant, I can immediately set $\lambda = 0$ so that $\nu = z$. Therefore as $h \rightarrow 0$ the *leading divergence* of the the orders of the Bessel functions in (54) is just that of their arguments and I can employ Nicholson's asymptotic relations. Starting from

$$\frac{2}{\pi z} R^{z,p}(z) = Y_z(z) J_{z+p+1}(z) - J_z(z) Y_{z+p+1}(z) \quad (63)$$

I need

$$\begin{aligned} Y_{z+\alpha}(z) &\sim 3^{-1/6} \left(\frac{\xi}{z}\right)^{1/3} [I_{1/3}(\xi) + I_{-1/3}(\xi)] \\ &= -\left(\frac{3}{x}\right)^{1/2} 3^{-1/6} \left(\frac{\xi}{z}\right)^{1/3} \text{Bi}(x) \end{aligned}$$

and

$$\begin{aligned} J_{z+\alpha}(z) &\sim \pi^{-1} 3^{-1/6} \left(\frac{\xi}{z}\right)^{1/3} K_{1/3}(\xi) \\ &= \left(\frac{3}{x}\right)^{1/2} 3^{-1/6} \left(\frac{\xi}{z}\right)^{1/3} \text{Ai}(x) \end{aligned}$$

where Ai and Bi are Airy functions and

$$\xi = \frac{2}{3} \left(\frac{2}{z}\right)^{1/2} \alpha^{3/2} = \frac{2}{3} x^{3/2}.$$

The parameter α is either 0 or $(p+1) = 1/h$ and $2/z = (hb)^3$ from which it is seen that the arguments, x , of the Airy functions are either 0 or b .

The multiplying factor reads

$$\left(\frac{3}{x}\right)^{1/2} 3^{-1/6} \left(\frac{\xi}{z}\right)^{1/3} = 3^{1/2} 3^{-1/6} \left(\frac{1}{z}\right)^{1/3} \left(\frac{2}{3}\right)^{1/3} = \left(\frac{2}{z}\right)^{1/3},$$

and there are two of these.

Hence we have the transitional limiting behaviour of the Lommel polynomials

$$\begin{aligned} R^{z,p}(z) &\sim \pi \left(\frac{z}{2}\right)^{1/3} (\text{Bi}(0) \text{Ai}(b) - \text{Ai}(0) \text{Bi}(b)) \\ &\sim \frac{1}{h} \frac{\pi}{b} (\text{Bi}(0) \text{Ai}(b) - \text{Ai}(0) \text{Bi}(b)). \end{aligned} \quad (64)$$

The form (64) contains within it Cauchy's limit,

$$J_\nu(\nu) \sim \frac{\Gamma(1/3)}{2^{2/3} 3^{1/6} \pi^{1/3} \nu^{1/3}},$$

and also

$$Y_\nu(\nu) \sim -\frac{3^{1/3} \Gamma(1/3)}{2^{2/3} \pi \nu^{1/3}}.$$

Numerically, choosing $p = 9$, a not too big a number, *i.e.* $h = 1/10$, the exact evaluation of $R(2000, 9, 2000)$ from the series is 10.84393086, for $b = 1$, whereas the limiting approximation, (64), gives 10.85339648. (These are just the same as the numbers in section (3).)

As I have not been too careful with normalisation, this quantity, (64), will be proportional to the functional determinant. This does not matter as I only want the *ratio* of the determinants, with and without b . As $b \rightarrow 0$, it is trivial to show that the right-hand side of (64) is just $1/(hb)$ and the desired ratio agrees with that, (23), obtained in the continuum directly by Kirsten and McKane, [12].

10. The discrete zero mode problem

If one of the eigenvalues, say λ_0 , vanishes, then the ordinary determinant is zero. It is then customary to calculate the product of the remaining non-zero eigenvalues and refer to this as the determinant. Kirsten and McKane, [12], give a modification of the Gel'fand Yaglom procedure that covers this case. Their formula just involves the zero mode eigenfunction. In this section I give the discrete version.

The result drops out of the discrete analogue of Green's theorem, or Lagrange's identity,¹⁴ or the Christoffel–Darboux identity, *e.g.* Atkinson, [5] §4.2. For speed, I copy the theorem from [5], for the recursion (1)

$$(\lambda - \mu) \sum_{j=1}^k y(j, \lambda) y(j, \mu) = \begin{vmatrix} y(k+1, \lambda) & y(k+1, \mu) \\ y(k, \lambda) & y(k, \mu) \end{vmatrix}, \quad 0 \leq k < p+1, \quad (65)$$

where λ and μ are any two numbers. Now choose μ to be an eigenvalue, λ_i , and set the upper limit $k = p$, the number of vertices. Then $y(p+1, \lambda)$ is the characteristic polynomial and so $y(p+1, \mu) = y(p+1, \lambda_i) = 0$. Equation (65) is rearranged into

$$\frac{y(p+1, \lambda)}{\lambda - \lambda_i} = \frac{1}{y(p, \lambda_i)} \sum_{j=1}^p y(j, \lambda) y(j, \lambda_i). \quad (66)$$

Setting λ to λ_i gives

$$\prod_{n \neq i} (\lambda_i - \lambda_n) = \frac{1}{y(p, \lambda_i)} \sum_{j=1}^p y(j, \lambda_i) y(j, \lambda_i) = -\frac{\langle y(\lambda_i) | y(\lambda_i) \rangle}{\Delta y(p, \lambda_i)} \quad (67)$$

¹⁴ This is the method employed in [12].

where I have again used the Dirichlet condition $y(p+1, \lambda_i) = 0$. Choosing $\lambda_i = \lambda_0 = 0$, the left-hand side is, up to a sign, the determinant, omitting the zero mode. This result should be compared with the relevant part of equation (14) in [12].

As a non-trivial example I again turn to the linear potential case when the characteristic polynomial is a Lommel polynomial. Specifically I choose 3 vertices ($p = 3$) and select the $\nu = -2$ root to give the zero mode. This means that the strength, B , has to equal -1 since $\nu = (2 - \lambda)/B$. The remaining two roots are then easily found as $\pm\sqrt{3}$ so that their determinant is -3 . Computation of the relevant Lommel polynomial, $R(-2, j-1)(-2)$, gives the zero mode as $(1, 1, -1)$, which is consistent with (67).

Incidentally, by dividing (66) and (67) one obtains Legendre's function and Legendre's polynomial interpolation of f can therefore be written as,

$$F(\lambda) = \sum_{n=0}^{p-1} f(\lambda_n) \frac{\langle y(\lambda) | y(\lambda_n) \rangle}{\langle y(\lambda_n) | y(\lambda_n) \rangle}, \quad (68)$$

in terms of a set of p orthogonal polynomials. (To repeat, the eigenvalues, λ_n , are the zeros of the polynomial, $y(p+1, \lambda)$.) An historic and practically important case corresponds to the free equation, $V = 0$, which yields Chebyshev polynomials. See [27] chap.6.

Equation (68) is related to a discrete Kramers sampling theorem, *cf* Annaby, [28]. If $f(\lambda)$ is a linear combination of the $y(j, \lambda)$, ($1 \leq j \leq p$), then $F(\lambda) = f(\lambda)$ and $f(\lambda)$ can be reconstructed from its samples, which is, perhaps, not surprising.

This can be more abstractly expressed as the vector space expansions,

$$|f\rangle = \sum_{j=1}^p |j\rangle \langle j | f \rangle = \sum_{n=0}^{p-1} \frac{|\lambda_n\rangle \langle \lambda_n | f \rangle}{\langle \lambda_n | \lambda_n \rangle}$$

(68) being regained on multiplying by $\langle \lambda |$, the function label, y , being suppressed. The condition on f corresponds to the bandwidth limitation of the original Whittaker-Shannon sampling theorem.

11. Comments

It might be said that the Bessel functions are only intermediaries in the calculation of the Lommel polynomials, which could be taken as the primary objects. Indeed, Bessel functions can be obtained as limits of Lommel polynomials, as shown

by Hurwitz, [29]. (Incidentally, precisely this limit was discussed by Bleich and Melan, [15], who make no reference to any earlier work.)

If this attitude is adopted, the form of the Lommel polynomials, *e.g.* (53), must be found without explicit use of Bessel functions, but using only the single recursion (37). Such is Lommel's original computation, [23], but he assumes the result and justifies it by induction which is somewhat synthetic. Bleich and Melan's method, [15], is interesting, but a little complicated, and again involves an assumption regarding the solution's general form. Graf and Gubler, [25] vol.2, however, use the recursion, expressed as a continued fraction, and obtain the Lommel polynomials, which they refer to as Schlöfli functions, directly. They list a few examples and also give the factored form (47).¹⁵

It is possible to derive any particular Lommel polynomial by direct iteration of the recursion (49), or (37). The reduction formula, [24], §26,

$$R^{\nu,p}(z) = \cos \frac{p\pi}{2} + \frac{2}{z} \sum_{s=0}^{p-1} (\nu + s + 1) \sin \frac{p-s}{2} \pi R^{\nu,s}$$

can also be iterated.

11. Conclusion

It has been shown that. apart from providing quite accurate approximations for smallish numbers of lattice points to a continuum situation, discrete techniques have an intrinsic interest and form a useful intro to the theory of orthogonal polynomials. In particular, I have highlighted the case of Lommel polynomials which seem to have been ignored. Even their general orthogonality properties do not seem to be available explicitly.

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¹⁵Although Watson, [26], is the undoubted Bessel bible, and Erdelyi, [30], the best summary of results, a number of earlier, and later, works, provide more detail and alternative approaches. I mention the rather attractive book by Nielsen, [24], which furnishes a more expansive treatment of the basics and contains results not available in [26]. A little referenced book is that by Graf and Gubler, [25], which presents the Schlöfli, complex integral, formulation of the theory. It is useful for the amount of algebraic detail given and also for Lommel polynomial properties. The pioneer work of Lommel, [23], is also valuable.

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